



Process/Equipment Co-Simulation: A Chemical Process Industry Perspective

Kunle Ogunde, P.E.
DuPont Titanium Technologies
Experimental Station
Wilmington, Delaware

**NETL 2009 Workshop on Advanced
Process Engineering Co-Simulation**
October 20, 2009

Agenda

- Motivation
- The challenges to adoption of Co-Simulation
- The TiO_2 Process as an example
 - Groundwork for critical mass
- Closing Thoughts

Motivation

- Highlight application challenges from the trenches
 - What can success deliver and what needs to be in place to make it happen?
- Address the question of whether Co-Simulation is merely bleeding edge technology waiting for applications or this is recent technology finally addressing *pre-existing* problems.
- Showcase a “how-to” vision that we in DuPont Titanium technologies are following that favors co-simulation and could enhance its success in the user community
- Spell out some potential issues with broad adoption of APECS technology.

Co-Simulation in Design versus Operations

- The case for Co-simulation in design flowsheets and for process optimization is perhaps a simple one.
 - In most instances, at least one CFD expert and an Aspen expert – very often not the same person - needed to implement.
 - Such collaboration is not unusual in large design or optimization project.
- The problem is the frequency of occurrence of these large design/optimization efforts.
 - The Chloride TiO_2 process is a classic case.
 - Highly model-centric
- The perspective of our DuPont Titanium Technologies modeling team is that the cost-benefit equation for co-simulation demands that the technology be robust enough for direct use in process operations support.

It's All About Economics...

- There was a time when corporations devoted large outlays to blue-sky research. That was then, this is now. DuPont CEO Ellen Kullman, calls it *The New Reality*.
 - More so than before, cost-benefit calculation is an up-front component behind most technical efforts – modeling included.
 - Globalization has drastically changed financial accountability principles at least in our company. We justify more, and work with less.
- This presents a huge opportunity for modeling to lower the overall cost of doing business especially if one adopts two forward-looking strategies
 - Use the right tool, and be open to integration of multiple tools
 - Follow an ancient proverb: *Dig your well before you're thirsty*

It's Also About the Support Structure for Modeling Technology

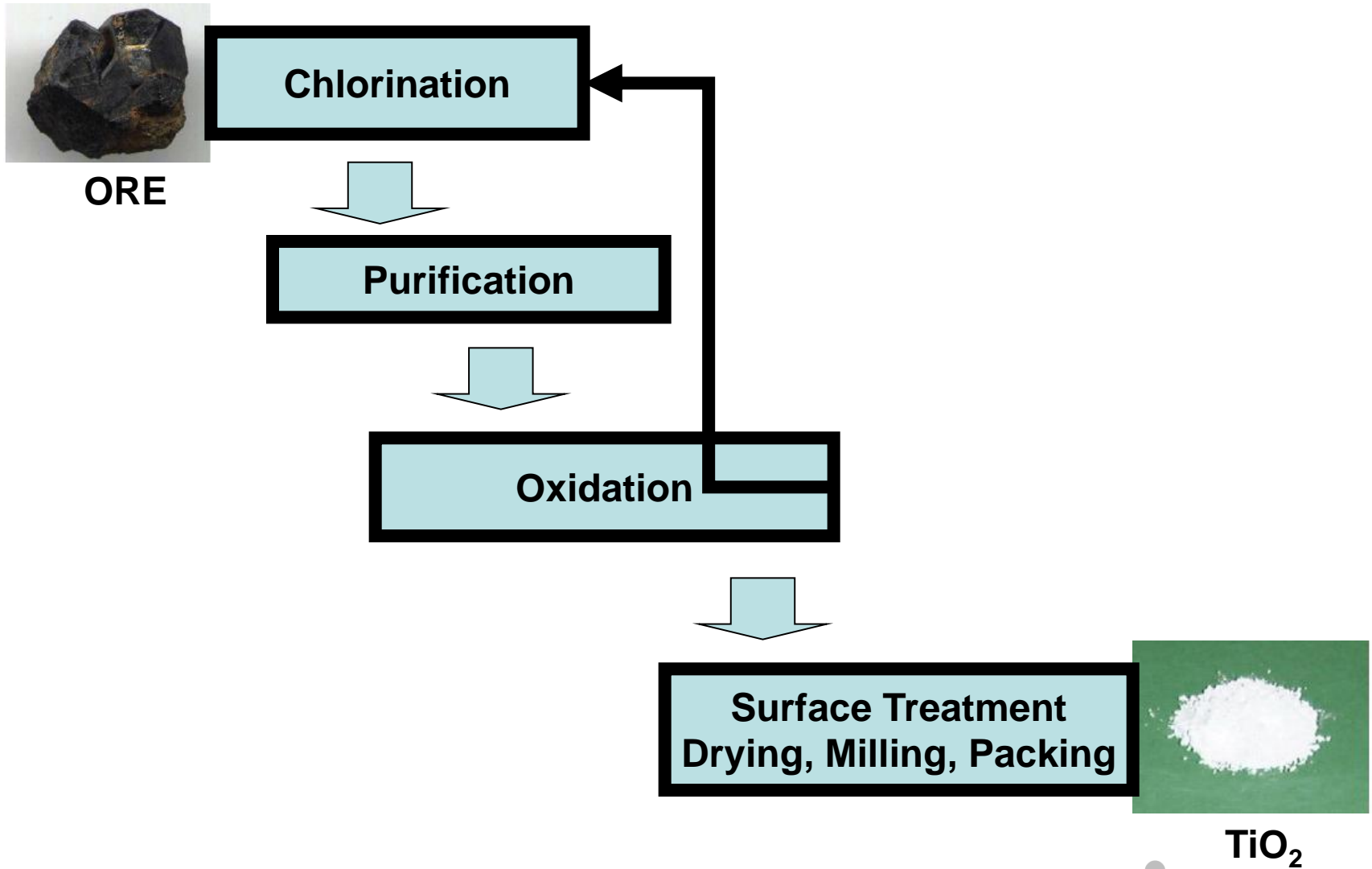
- Organizational structure can stifle the use patterns of models
 - For design, it's clear what needs to be done and what organizational structure we need
 - For the overwhelming number of application scenarios, it's not so clear
 - Models tend to be used re-actively rather than pro-actively: do enough to fight the current fire versus build an enduring digitally simulated analog for the physical plant!
 - In larger companies with the resource depth: modeling is done in distributed centers of concentrated expertise. The model, or more likely, the model output, then flows down to the end user(s).
 - The problem: Rarely does that *leveraged* expert model developer maintain a continuing link and sense of ownership to the developed models in a way that promotes optimum value extraction.
- Overcoming this productivity leak is one of the challenges before a technology like co-simulation. It really needs to be lined up as a ready tool in an integrated modeling approach.

The DuPont Titanium Technologies Example

● Ingredients for Success

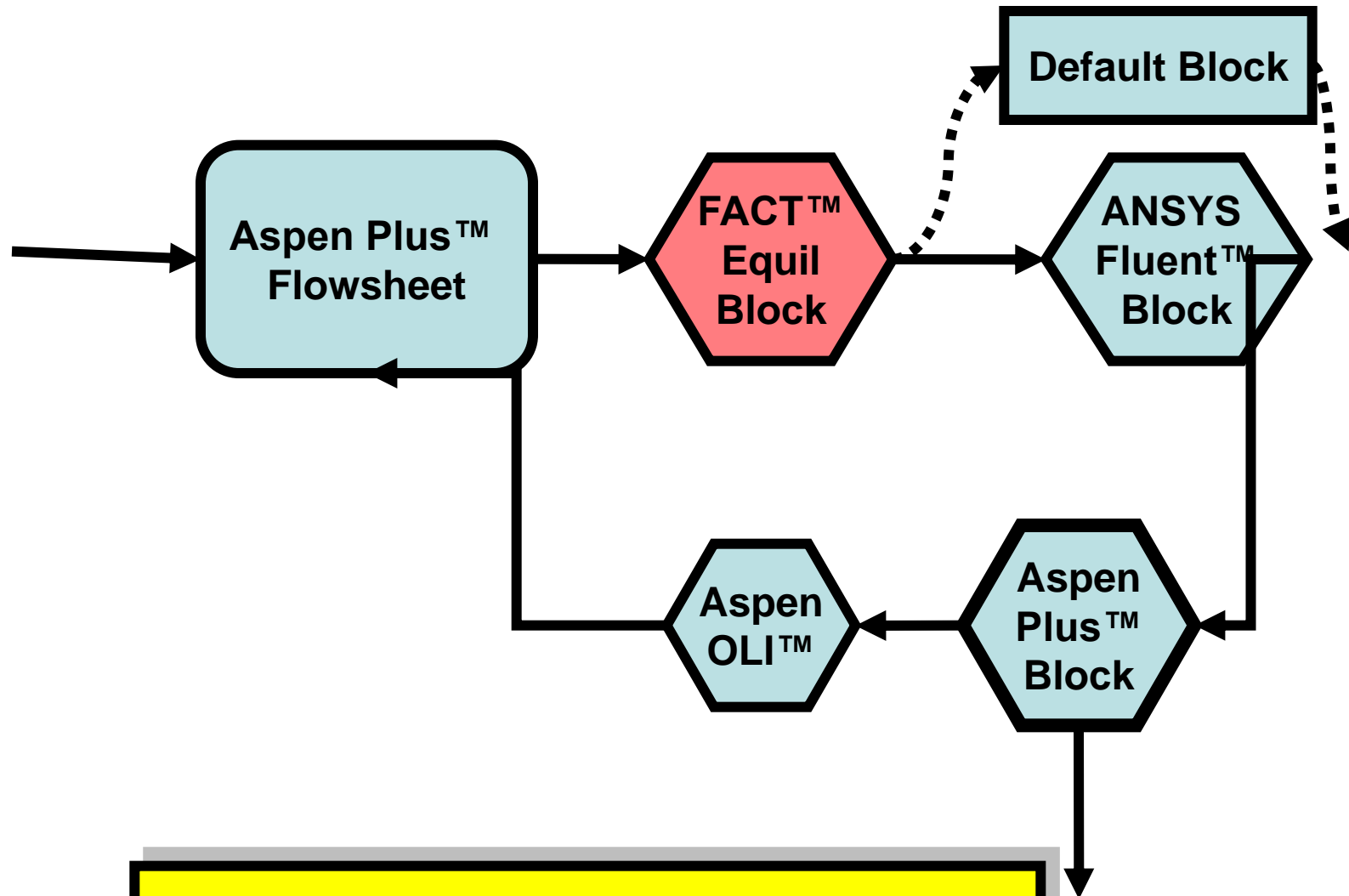
- A single standing team with a common, broad-based goal of modeling one of the most complex, model-centric processes there is in the DuPont toolbox.
- Availability of experts with islands of expertise
 - typically applied in stand-alone or per incident fashion – but available nonetheless.
- A vision of what is possible given the confluence of technology advancement – in both software and hardware.
- The business driver: a very mature, very complex process that demands creativity to remain sustainable and profitable.

Chloride TiO_2 Process Technology



The phase history and transitions in the Chloride TiO_2 Process make a compelling case for Co-Simulation blocks

An Illustration of the Structure of an Integrated Modeling Environment Based on an Aspen Backbone



Drivers for Co-Simulation

- The promise of computation hardware: higher speed, higher capacity
- The incredible level of inter-operability now evident in the most widely used modeling tools
- Inter-operability and scalability of computing resources
- The process environment is very hostile to measurement systems. There is then value to calculating that which cannot be **easily** or **cost-effectively** measured. Often a 1-D flowsheet is all it takes. But the ability to call on Co-Simulation tools opens the door wider to innovation.

APECS Co-Simulation is similar to constructing process equipment and piping with transparent material!

Drivers for Modeling the Process

- The characteristics of the Chloride Process
 - Multiphase equilibria
 - Very fast homogenous and heterogenous reactions
 - Mixing issues
 - Very challenging measurement environment for all but the most specialized sensors (making model validation a challenge by itself)
 - Extremes of temperature
 - Very complicated nested process loops that are hard to converge during modeling
 - Large component list – essentially the Periodic Table – because the feedstock is naturally occurring.
- Sustainability and environmental footprint reduction in line with the mission of the DuPont Corporation

Co-Simulation Testing in TiCl_4 Oxidation

- We tested APECS in 2006 to simulate a 5-m section of a medium-sized Aspen Plus flowsheet of TiCl_4 Oxidation (about 60-70 Aspen blocks).
- Runs were carried on a Dell Windows XP workstation running Fluent 6.x and Aspen Plus 2004.x.
- We made several simplifications:
 - Used a 2-D Fluent model in place of the 3-D model we originally started with (for speed)
 - Opted to model a line with no recycle around the Co-Simulation block.
 - Even though desirable for the case in point, we did not add a second Fluent block because Fluent at the time required the same number of licenses as Fluent blocks even though the flowsheet is sequential modular.

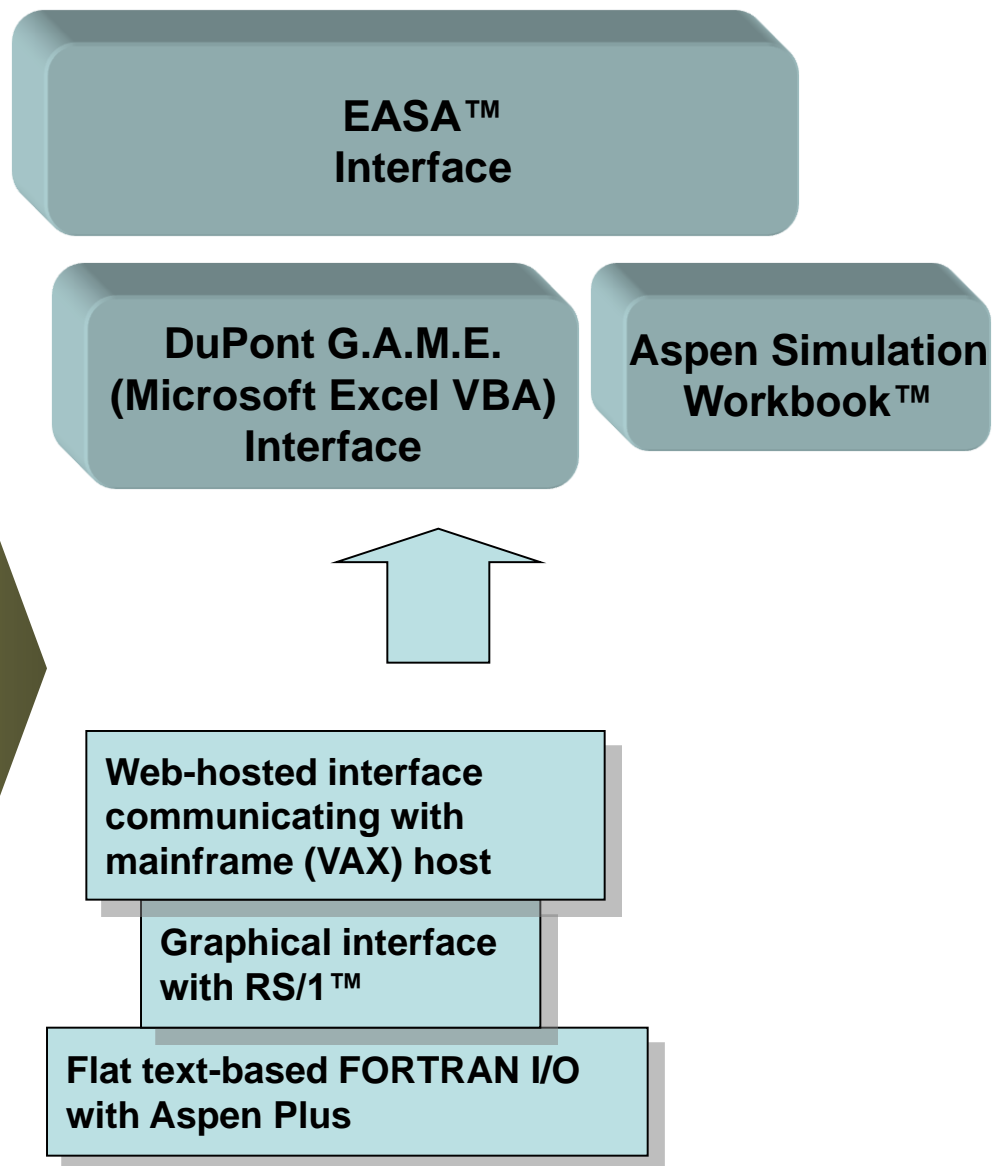
APECS Test Results

- Overall, the test was successful but we also encountered our fair share of early adopter configuration problems not unexpected with such a complex venture.
- There also were some underlying challenges with the Aspen flowsheet stemming from our vision of how, and by whom, the flowsheet would be ultimately used.
- Observations & Decisions
 - For our TiCl_4 Oxidation model implementation, we found that we didn't have a seamless way to make the inclusion of the APECS block user-selectable at run-time
 - Held off further development with APECS to allow for:
 - product maturity and robustness to improve
 - Solution of the problem of excessive consumption of Fluent licenses for multiple instances of APECS in a model .
 - Decided to seek/develop technology to open access to these models to the larger technical community of non-experts in the TiO_2 business who would ordinarily be incapable of running models at this level of complexity.
 - Focus on addressing issues we had with implementing Aspen Hierarchy blocks: a task that we consider a component of an overall strategy for deploying and supporting Aspen flowsheets with, and without, co-simulation.

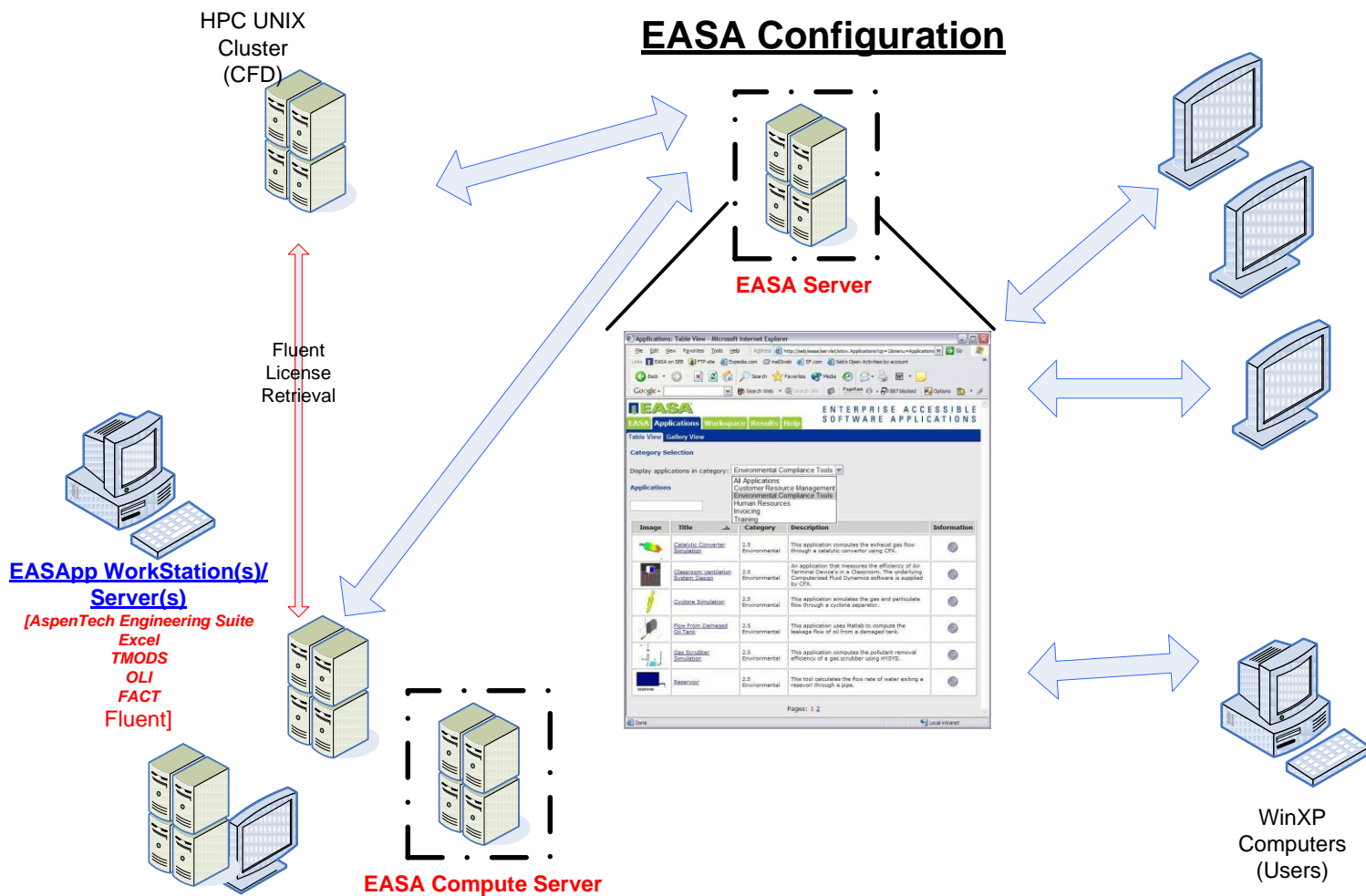
Building Blocks for An Easy Access Platform

Goals

- Create comprehensive models of process sections assembled from existing smaller models of process equipment and flowsheets.
- Maintain flexibility to continue independent development and upgrade of the constituent models, allowing for seamless drop-in and re-integration of updated versions as deemed necessary.
- Add usability features – especially I/O – to vastly expand the user base.



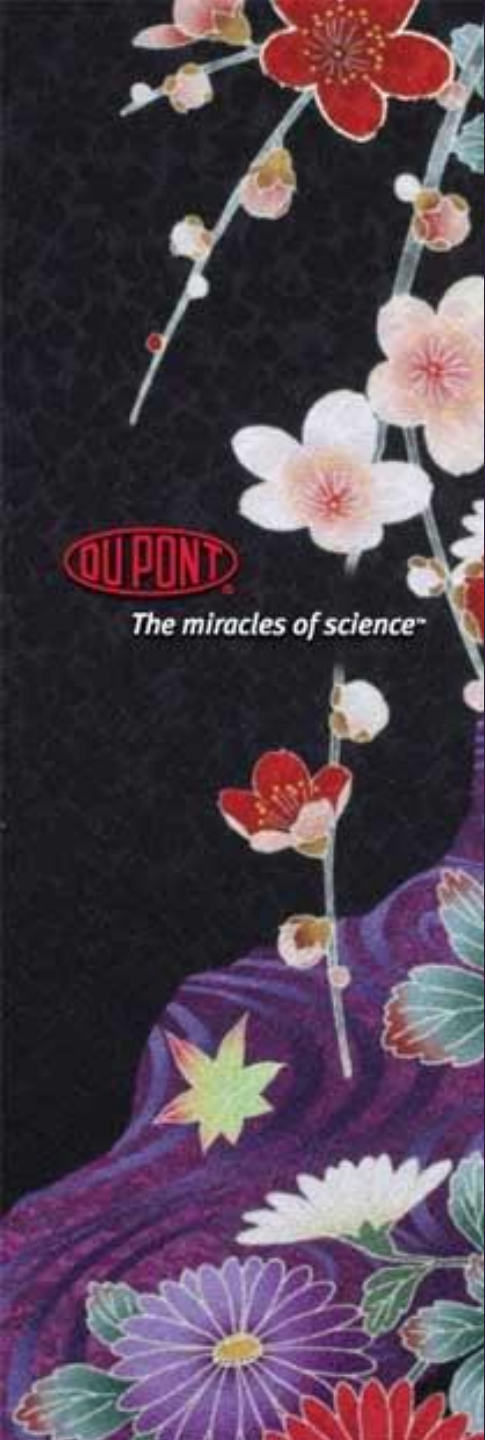
Cloud Computing Modeling Platform



EASA is a trademark of EASA Software (www.easasoftware.com)

Closing Thoughts

- Even our limited experience with co-simulation confirms that, especially for processes that are generally unfriendly to measurement sensors, it has the potential to provide detailed windows we wouldn't otherwise have. It may find more use in design applications right now, but we see even stronger potential for its use in troubleshooting, routine process optimization and for developing better process understanding.
- Such potential cannot be fulfilled when the co-simulation tool is used or usable only in the occasional, rare application. Hence conscious effort must be made to fit the technology into the latest modeling framework that everybody from AspenTech to ANSYS has embraced: robust inter-operability is a must and versatile configuration tools should make integration into small and large models relatively easy.
- The ease of integration is especially critical because the return on investment for co-simulation will be better guaranteed by a larger set of application possibilities.
- In the modeling community at large, application habits may need to undergo a drastic change; advanced hardware at our disposal is a necessary challenge to our creativity to get more with less effort, and less manpower. But this is only possible if inter-operability is as important in the planning process as it should be.
- Our models are currently all Sequential Modular in large part because Aspen (2006.5 and below) does not natively support multiphase models with solids in the Equation-Oriented mode. Consequently, run duration of these models can sometimes be quite long. The question for the future is: How would APECS work in an Equation-Oriented model?



Questions?